Nithiamide

140-40-9 | DTXSID6046391

## Model Performance

| Model | Data |
|---|---|

### Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

## Model Results

**Predicted value:** 9.16e-12 cm3/molecule*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 1.98e-01

**Confidence level:** 6.14e-01

## Nearest Neighbors from the Training Set

Image not found
Dimethyl adipate
**Measured:** 8.40e-12
**Predicted:** 6.84e-12

Image not found
Dimethyl glutarate
**Measured:** 3.30e-12
**Predicted:** 3.76e-12

Image not found
2(3H)-Furanone
**Measured:** 4.45e-11
**Predicted:** 3.74e-11

Image not found
2,5-Furandione
**Measured:** 1.45e-12
**Predicted:** 2.17e-12